

Ethyl hydrogen glutarate  
1070-62-8 | DTXSID20147865

Model Performance

|       |      |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.95            | 0.69 | 0.95           | 0.65 | 0.96       | 0.68 |

Model Results

Predicted value: 6.30

Global applicability domain: Inside

Local applicability domain index: 7.42e-01

Confidence level: 4.19e-01

Nearest Neighbors from the Training Set

|  |  |   |
|--|--|---|
| <div>Image not found</div> <div>1-Octanol</div> <div>Measured: 6.03</div> <div>Predicted: 5.95</div> | <div>Image not found</div> <div>Methylparaben</div> <div>Measured: 8.57</div> <div>Predicted: 7.06</div> | <div>Image not found</div> <div>Cyclohexanol</div> <div>Measured: 5.18</div> <div>Predicted: 4.72</div> |
| <div>Image not found</div> <div>1-Hexanol</div> <div>Measured: 5.18</div> <div>Predicted: 4.67</div> | <div>Image not found</div> <div>Dipropylamine</div> <div>Measured: 3.59</div> <div>Predicted: 4.37</div> |   |